# Contents to volume 100

## Computational physics

Track fitting with non-Gaussian noise	1
Bajpai, R.P. and S.N. Rai Behavior of two, three and four site states self-interacting neural networks	17
Tennyson, J.  Phase factors in electron-molecule collision calculations	26
Thomas, Jr., E., G.E. Sasser, S.F. Knowlton, J.D. Hanson and R.F. Gandy A new technique for calculating toroidal harmonic coefficients for curl-free magnetic fields in helical toroidal devices	31
McCoy, R.A. and Y. Deng Parallel embedded-atom method simulations with delayed electron density approximations	41
Jost, G., T.M. Tran, K. Appert and S. Wüthrich Effects of electron-cyclotron instabilities on gyrotron beam quality	47
Ixaru, L.Gr., G. Vanden Berghe, H. De Meyer and M. Van Daele Four-step exponential-fitted methods for nonlinear physical problems	56
Roberts, A.J.  Low-dimensional modelling of dynamics via computer algebra	215
del Aguila, F., J.A. Aguilar-Saavedra and M. Zrałek Invariant analysis of CP violation	231
Bérces, A., R.M. Dickson, L. Fan, H. Jacobsen, D. Swerhone and T. Ziegler An implementation of the coupled perturbed Kohn-Sham equations: perturbation due to nuclear displacements	247
Jacobsen, H., A. Bérces, D.P. Swerhone and T. Ziegler Analytic second derivatives of molecular energies: a density functional implementation	263
Computer programs in physics	
Ixaru, L.Gr., H. De Meyer, G. Vanden Berghe and M. Van Daele EXPFIT4 – a FORTRAN program for the numerical solution of systems of nonlinear second-orde initial-value problems	r 7
Jönsson, P. and C. Froese Fischer SMS92: a program for relativistic isotope shift calculations	8

# Contents to volume 100

## Computational physics

Track fitting with non-Gaussian noise	1
Bajpai, R.P. and S.N. Rai Behavior of two, three and four site states self-interacting neural networks	17
Tennyson, J.  Phase factors in electron-molecule collision calculations	26
Thomas, Jr., E., G.E. Sasser, S.F. Knowlton, J.D. Hanson and R.F. Gandy A new technique for calculating toroidal harmonic coefficients for curl-free magnetic fields in helical toroidal devices	31
McCoy, R.A. and Y. Deng Parallel embedded-atom method simulations with delayed electron density approximations	41
Jost, G., T.M. Tran, K. Appert and S. Wüthrich Effects of electron-cyclotron instabilities on gyrotron beam quality	47
Ixaru, L.Gr., G. Vanden Berghe, H. De Meyer and M. Van Daele Four-step exponential-fitted methods for nonlinear physical problems	56
Roberts, A.J.  Low-dimensional modelling of dynamics via computer algebra	215
del Aguila, F., J.A. Aguilar-Saavedra and M. Zrałek Invariant analysis of CP violation	231
Bérces, A., R.M. Dickson, L. Fan, H. Jacobsen, D. Swerhone and T. Ziegler An implementation of the coupled perturbed Kohn-Sham equations: perturbation due to nuclear displacements	247
Jacobsen, H., A. Bérces, D.P. Swerhone and T. Ziegler Analytic second derivatives of molecular energies: a density functional implementation	263
Computer programs in physics	
Ixaru, L.Gr., H. De Meyer, G. Vanden Berghe and M. Van Daele EXPFIT4 – a FORTRAN program for the numerical solution of systems of nonlinear second-orde initial-value problems	r 7
Jönsson, P. and C. Froese Fischer SMS92: a program for relativistic isotope shift calculations	8

### Contents to volume 100

Jemmer, P. and P.J. Knowles

Program index to volume 100

323

326

Generation of functional derivatives in Kohn-Sham density-functional theory

Caffo, M. and H. Czyż

BHAGEN-1PH: a Monte Carlo event generator for radiative Bhabha scattering

Hernández, J.J. and S. Navas

JASP: a program to estimate discovery and exclusion limits in prospective studies of searches

119

Fujimoto, J., T. Ishikawa, T. Kaneko, K. Kato, S. Kawabata, Y. Kurihara, T. Munehisa, D. Perret-Gallix, Y. Shimizu and H. Tanaka

grc4f v1.1: a four-fermion event generator for e<sup>+</sup>e<sup>-</sup> collisions

128

Ayari, M.A. and V. Hussin

GLie: a MAPLE program for Lie supersymmetries of Grassmann-valued differential equations

157

Hartley, D.

EDS: A REDUCE package for exterior differential systems

177

Arneodo, M., L. Lamberti and M. Ryskin

DIPSI: a Monte Carlo generator for elastic vector meson production in charged lepton-proton
scattering

195

Popowicz, Z.
S U S Y 2

Demetriou, I.C.

CXFTV2: A Fortran subroutine for the discrete least squares convex approximation 297

Häkkinen, J. and H. Kharraziha
Colour: a computer program for QCD colour factor calculations
311

Contents to volume 100 322
Author index to volume 100 324